

Modeling primary breakup: A three-dimensional Eulerian level set/vortex sheet method for two-phase interface dynamics

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1. Motivation and objectives

Atomization processes play an important role in a wide variety of technical applications and natural phenomena, ranging from inkjet printers, gas turbines, direct injection IC-engines, and cryogenic rocket engines to ocean wave breaking and hydrothermal features. The atomization process of liquid jets and sheets is usually divided into two consecutive steps: the primary and the secondary breakup. During primary breakup, the liquid jet or sheet exhibits large scale coherent structures that interact with the gas-phase and break up into both large and small scale drops. During secondary breakup, these drops break up into ever smaller drops that finally may evaporate.

Usually, the atomization process occurs in a turbulent environment, involving a wide range of time and length scales. Given today's computational resources, the direct numerical simulation (DNS) of the turbulent breakup process as a whole, resolving all physical processes, is impossible, except for some very simple configurations. Instead, models describing the physics of the atomization process have to be employed.

Various models have already been developed for the secondary breakup process. There, it can be assumed that the characteristic length scale ℓ of the drops is much smaller than the available grid resolution Δx and that the liquid volume fraction in each grid cell Θ_l is small, see Fig. 1. Furthermore, assuming simple geometrical shapes of the individual drops, like spheres or ellipsoids, the interaction between these drops and the surrounding fluid can be taken into account. Statistical models describing the secondary breakup process in turbulent environments can thus be derived (O'Rourke 1981; O'Rourke & Amsden 1987; Reitz 1987; Reitz & Diwakar 1987; Tanner 1997).

However, the above assumptions do not hold true for the primary breakup process. Here, the turbulent liquid fluid interacts with the surrounding turbulent gas-phase on scales larger than Δx , resulting in highly complex interface dynamics and individual grid cells that can be fully immersed in the liquid phase, compare Fig. 1. An explicit treatment of the phase interface and its dynamics is therefore required. To this end, we propose to follow in essence a Large Eddy Simulation (LES) type approach: all interface dynamics and physical processes occurring on scales larger than the available grid resolution Δx shall be fully resolved and all dynamics and processes occurring on subgrid scales shall be modeled. The resulting approach is called Large Surface Structure (LSS) model.

In order to develop such a LSS model for the turbulent primary breakup process, one potential approach is to start off from a fully resolved description of the interface dynamics using the Navier-Stokes equations and include an additional source term in the momentum equation due to surface tension forces (Brackbill *et al.* 1992). In order to track the location, motion, and topology of the phase interface, the Navier-Stokes equations are then coupled to one of various possible tracking methods, for example marker particles

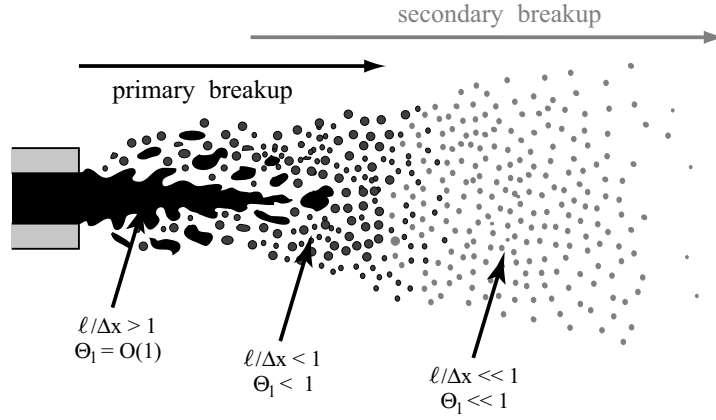


FIGURE 1. Breakup of a liquid jet.

(Brackbill *et al.* 1988; Rider & Kothe 1995; Unverdi & Tryggvason 1992), the Volume-of-Fluid method (Noh & Woodward 1976; Kothe & Rider 1994; Gueyffier *et al.* 1999), or the level set method (Osher & Sethian 1988; Sussman *et al.* 1994, 1998). Then, introducing ensemble averaging or spatial filtering results in unclosed terms that require modeling (Brocchini & Peregrine 2001*a,b*). Unfortunately, the derivation of such closure models is not straightforward and, hence, has not been achieved yet. This is in part due to the fact that, with the exception of the surface tension term, all other physical processes occurring at the phase interface itself, like for example stretching, are not described by explicit source terms. Instead, they are hidden within the interdependence between the Navier-Stokes equations and the respective interface tracking equation. Thus, a formulation containing the source terms explicitly could greatly facilitate any attempt to derive the appropriate closure models.

To this end, a novel three-dimensional Eulerian level set/vortex sheet method is proposed. Its advantage is the fact that it contains explicit source terms for each individual physical process that occurs at the phase interface. It thus constitutes a promising framework for the derivation of the LSS subgrid closure models.

This paper is divided into four parts. First, the level set/vortex sheet method for three-dimensional two-phase interface dynamics is presented. Second, the LSS model for the primary breakup of turbulent liquid jets and sheets is outlined and all terms requiring subgrid modeling are identified. Then, preliminary three-dimensional results of the level set/vortex sheet method are presented and discussed. Finally, conclusions are drawn and an outlook to future work is given.

2. The level set/vortex sheet method

The aim of the level set/vortex sheet method is to describe the dynamics of the phase interface Γ between two inviscid, incompressible fluids 1 and 2, as shown in Fig. 2. In this case, the velocity $\mathbf{u}_i$ on either side i of the interface Γ is determined by the incompressible Euler equations, given here in dimensionless form,

$$\nabla \cdot \mathbf{u}_i = 0, \quad (2.1)$$

$$\frac{\partial \mathbf{u}_i}{\partial t} + (\mathbf{u}_i \cdot \nabla) \mathbf{u}_i = -\frac{1}{\rho_i} \nabla p, \quad (2.2)$$

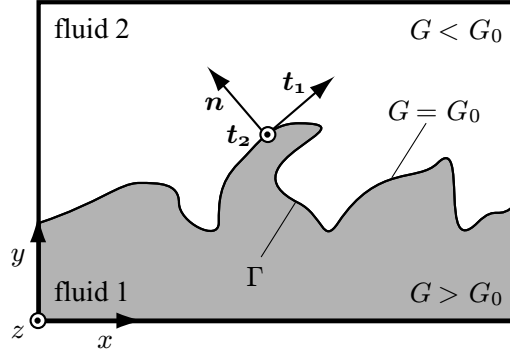


FIGURE 2. Phase interface definition.

subjected to the boundary conditions at the interface Γ ,

$$[(\mathbf{u}_1 - \mathbf{u}_2) \cdot \mathbf{n}] \Big|_{\Gamma} = 0 \quad (2.3)$$

$$[\mathbf{n} \times (\mathbf{u}_2 - \mathbf{u}_1)] \Big|_{\Gamma} = \boldsymbol{\eta} \quad (2.4)$$

$$[p_2 - p_1] \Big|_{\Gamma} = \frac{1}{\text{We}} \kappa \quad (2.5)$$

and at infinity,

$$\lim_{y \rightarrow \pm\infty} \mathbf{u}_i = \pm \mathbf{u}_{\infty} . \quad (2.6)$$

Here, $\mathbf{n}$ is the interface normal vector, $\boldsymbol{\eta}$ is the vortex sheet strength, and κ is the local curvature of Γ . The Weber number is defined as

$$\text{We} = \rho_{\text{ref}} u_{\text{ref}}^2 / \Sigma L_{\text{ref}} , \quad (2.7)$$

where Σ is the surface tension coefficient and ρ_{ref} , u_{ref} , and L_{ref} are the reference density, velocity, and length, respectively. An interface subjected to the above boundary conditions is called a vortex sheet (Saffman & Baker 1979).

The partial differential equation describing the evolution of the vortex sheet strength $\boldsymbol{\eta}$ can be derived by combining the Euler equations, Eqs. (2.1) and (2.2), with the boundary conditions at the interface, Eqs. (2.3)-(2.5), resulting in (Pozrikidis 2000)

$$\begin{aligned} \frac{\partial \boldsymbol{\eta}}{\partial t} + \mathbf{u} \cdot \nabla \boldsymbol{\eta} = & -\mathbf{n} \times [(\boldsymbol{\eta} \times \mathbf{n}) \cdot \nabla \mathbf{u}] + \mathbf{n} [(\nabla \mathbf{u} \cdot \mathbf{n}) \cdot \boldsymbol{\eta}] \\ & + \frac{2(A+1)}{\text{We}} (\mathbf{n} \times \nabla \kappa) + 2A \mathbf{n} \times \mathbf{a} . \end{aligned} \quad (2.8)$$

Here, $A = (\rho_1 - \rho_2)/(\rho_1 + \rho_2)$ is the Atwood number and $\mathbf{a}$ is the average acceleration of fluid 1 and fluid 2 at the interface. The major advantage of Eq. (2.8), as compared to a formulation based on the Euler equations, is the fact that Eq. (2.8) contains explicit local individual source terms on the right-hand side describing the physical processes at the interface. These are, from left to right, two stretching terms, a surface tension term $\mathbf{T}_{\sigma}$, and a density difference term.

In addition to the evolution of the local vortex sheet strength, Eq. (2.8), the location and motion of the phase interface itself has to be known. To this end, vortex sheets are typically solved by a boundary integral method within a Lagrangian framework where the phase interface is tracked by marker particles (Baker *et al.* 1982; Pullin 1982; Hou

et al. 1997, 2001; Rangel & Sirignano 1988). Marker particles allow for highly accurate tracking of the phase interface motion in a DNS. However, the introduction of ensemble averaging and spatial filtering of the interface topology is not straightforward and hence a strategy for the derivation of appropriate LSS subgrid closure models is not directly apparent.

Level sets, on the other hand, have been successfully applied to the derivation of closure models in the field of premixed turbulent combustion (Peters 1999, 2000). Thus, instead of using marker particles to describe the location and motion of the phase interface, here, the interface is represented by an iso-surface of the level set scalar field $G(\mathbf{x}, t)$, as shown in Fig. 2. Setting

$$G(\mathbf{x}, t)|_{\Gamma} = G_0 = \text{const}, \quad (2.9)$$

$G(\mathbf{x}, t) > G_0$ in fluid 1, and $G(\mathbf{x}, t) < G_0$ in fluid 2, an evolution equation for the scalar G can be derived by simply differentiating Eq. (2.9) with respect to time,

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = 0. \quad (2.10)$$

This equation is called the level set equation (Osher & Sethian 1988). Using the level set scalar, geometrical properties of the interface, like its normal vector and curvature, can be easily expressed as

$$\mathbf{n} = \frac{\nabla G}{|\nabla G|}, \quad \kappa = \nabla \cdot \mathbf{n}. \quad (2.11)$$

Strictly speaking, Eqs. (2.8) and (2.10) are valid only at the location of the interface itself. However, to facilitate the numerical solution of both equations in the whole computational domain, $\boldsymbol{\eta}$ is set constant in the interface normal direction,

$$\nabla \boldsymbol{\eta} \cdot \nabla G = \mathbf{0}, \quad (2.12)$$

and G is chosen to be a distance function away from the interface,

$$|\nabla G| \Big|_{G \neq G_0} = 1. \quad (2.13)$$

Equations (2.8) and (2.10) are coupled by the self-induced velocity $\mathbf{u}$ of the vortex sheet. To calculate $\mathbf{u}$, the vector potential $\boldsymbol{\psi}$ is introduced,

$$\Delta \boldsymbol{\psi} = \boldsymbol{\omega}. \quad (2.14)$$

Here, the vorticity vector $\boldsymbol{\omega}$ is calculated following a vortex-in-cell type approach (Christiansen 1973; Cottet & Koumoutsakos 2000)

$$\boldsymbol{\omega}(\mathbf{x}) = \int_V \boldsymbol{\eta}(\mathbf{x}') \delta(\mathbf{x} - \mathbf{x}') \delta(G(\mathbf{x}') - G_0) |\nabla G(\mathbf{x}')| d\mathbf{x}', \quad (2.15)$$

where δ is the delta-function. Then, $\mathbf{u}$ can be calculated from

$$\mathbf{u}(\mathbf{x}) = \int_V \delta(\mathbf{x} - \mathbf{x}') (\nabla \times \boldsymbol{\psi}) d\mathbf{x}'. \quad (2.16)$$

In summary, Eqs. (2.8), (2.10), and (2.14) - (2.16) describe the three-dimensional two-phase interface dynamics and constitute the level set/vortex sheet method.

2.1. Numerical methods

Numerically, Eqs. (2.8) and (2.10) are solved in a narrow band (Peng *et al.* 1999) by a third-order WENO scheme (Jiang & Peng 2000) using a third-order TVD Runge-

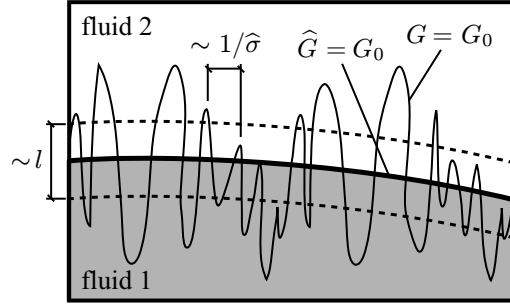


FIGURE 3. LSS interface definitions.

Kutta time discretization (Shu & Osher 1989). The redistribution of $\boldsymbol{\eta}$ (2.12) is solved by a Fast Marching Method (Sethian 1996; Adalsteinsson & Sethian 1999), whereas the reinitialization of G (2.13) is solved by an iterative procedure (Sussman *et al.* 1994; Peng *et al.* 1999). The interested reader is referred to Herrmann (2002) for a detailed description of the numerical methods employed in the level set/vortex sheet method.

3. The LSS model for turbulent primary breakup

The basic idea of the LSS model is to split the treatment of the primary breakup process into two parts. All phase interface dynamics occurring on scales larger than the local grid size are explicitly resolved and tracked by a level set approach, whereas interface dynamics occurring on subgrid scales are described by an appropriate subgrid model. Furthermore, the LSS subgrid model has to separate out all broken off subgrid scale liquid drops and transfer them to a secondary breakup model.

The level set equation describing the interface location and motion on the resolved scales can be derived by first introducing appropriate interface based filters (Oberlack *et al.* 2001) into the level set equation (2.10), see Fig. 3,

$$\frac{\partial \hat{G}}{\partial t} + \hat{\mathbf{u}} \cdot \nabla \hat{G} = 0. \quad (3.1)$$

Here, $\hat{\cdot}$ denotes quantities on the resolved (filter) scale. Furthermore, the mass transfer rate $\dot{m}_p$ into the secondary breakup model has to be taken into account,

$$\dot{m}_p = \rho_1 s_p \hat{A}_{G_0} = \frac{4}{3} \pi \rho_1 \frac{\partial}{\partial t} \int_0^{\Delta x} P(D) D^3 dD, \quad (3.2)$$

where s_p is the subgrid primary breakup velocity, $\hat{A}_{G_0}$ is the local surface area of the resolved interface, and $P(D)$ is the droplet diameter number distribution,

$$\int_0^\infty P(D) dD = N, \quad (3.3)$$

where N is the total number of drops. Then, the resolved scale level set equation reads

$$\frac{\partial \hat{G}}{\partial t} + (\hat{\mathbf{u}} + s_p \hat{\mathbf{n}}) \cdot \nabla \hat{G} = 0, \quad (3.4)$$

where $\hat{\mathbf{n}}$ is the normal vector of the resolved scale interface,

$$\hat{\mathbf{n}} = \frac{\nabla \hat{G}}{|\nabla \hat{G}|}. \quad (3.5)$$

To describe the phase interface dynamics on the resolved scale, their effect on the flow field has to be taken into account by an additional source term $\mathbf{T}$ in the momentum equation,

$$\mathbf{T} = \Sigma \hat{\kappa} \delta(\hat{G} - G_0) \hat{\mathbf{n}} + \mathbf{T}_{\text{SGS}}. \quad (3.6)$$

Here, the first term on the right-hand side describes the effect of surface tension forces due to the local curvature $\hat{\kappa}$ of the resolved scale interface, whereas the second term, $\mathbf{T}_{\text{SGS}}$, accounts for the effect of the subgrid scale surface tension forces on the resolved scale flow field.

Thus, the yet unclosed subgrid terms of the LSS model requiring modeling are the subgrid primary breakup velocity s_p , the droplet diameter number distribution $P(D)$, and the subgrid scale surface tension effect $\mathbf{T}_{\text{SGS}}$. As previously indicated, these subgrid terms are to be derived from the level set/vortex sheet method. Performing DNS of the primary breakup of liquid surfaces and sheets in turbulent environments will help to identify characteristic regimes of the turbulent primary breakup and their dominant physical processes. These can then be quantified using the explicit source terms in the $\boldsymbol{\eta}$ -equation (2.8), thus providing guidelines for the derivation of appropriate LSS subgrid models.

4. Results

In order to both validate the three-dimensional level set/vortex sheet method and to demonstrate its ability to perform DNS of the primary breakup process, the results of two different cases are presented. First, the calculated oscillation periods of liquid columns and spheres are compared to theoretical results. Then, the breakups of a randomly perturbed liquid surface and sheet are presented.

4.1. Oscillating columns and spheres

To validate the proposed level set/vortex sheet method, the calculated oscillation periods T of liquid columns and spheres of mean radius $R = 0.25$, center $\mathbf{x}_c = (0.5, 0.5, 0.5)$, amplitude $\epsilon = 0.05R$, and Atwood number $A = 0$ are compared to theoretical results (Lamb 1945). The initial vortex sheet strength in both cases is set to

$$\boldsymbol{\eta}(\mathbf{x}, t = 0) = \mathbf{0}. \quad (4.1)$$

All calculations are performed in a unit sized box resolved by an equidistant cartesian grid of 128×128 and $128 \times 128 \times 128$ nodes, respectively.

Figure 4 shows the distribution of the surface tension term $\mathbf{T}_\sigma$ of the $\boldsymbol{\eta}$ -equation (2.8) in the x -, y -, and z -direction,

$$\mathbf{T}_\sigma = \frac{2(A+1)}{\text{We}} (\mathbf{n} \times \nabla \kappa), \quad (4.2)$$

for the oscillating sphere of mode number $n = 5$ and Weber number $\text{We} = 10$ calculated at $t = 0$. As the shape of the sphere indicates, $\mathbf{T}_\sigma$ in the x -direction is a factor of roughly four higher than $\mathbf{T}_\sigma$ in the other two directions, leading to the predominant oscillation in the y - z -plane.

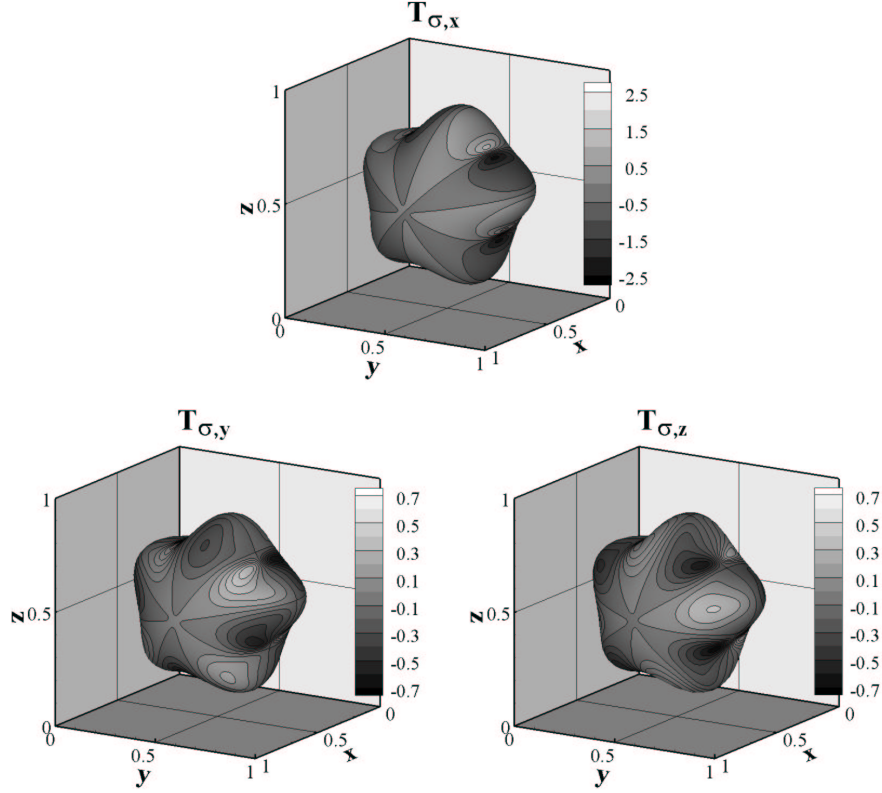


FIGURE 4. Distribution of the surface tension term T_σ in the x -direction (top), y -direction (left), and z -direction (right) for the mode $n = 5$ oscillating sphere at $t = 0$ and $We = 10$.

Figure 5 depicts the comparison of the oscillation period for the oscillating columns on the left-hand side and the oscillating spheres on the right-hand side for two different Weber numbers. As can be clearly seen, agreement between simulation and theory is very good.

4.2. Liquid surface and sheet breakup

To demonstrate the capability of the proposed level set/vortex sheet method to simulate the primary breakup process, the temporal evolution of both a randomly perturbed liquid surface and sheet are simulated. In the case of the liquid surface, the on average flat interface located at $z = 0$ is perturbed in the z -direction by a Fourier series of 64 sinusoidal waves in both the x - and y -direction with random amplitude $0 < \epsilon < 0.01$ and random phase shift. In the case of the liquid sheet, the two on average flat interfaces are located at $z = -B/2$ and $z = +B/2$ and are again perturbed by two Fourier series of 64 sinusoidal waves. The thickness of the liquid sheet is set to $B = 0.1$.

The initial vortex sheet strength for the liquid surface is set to

$$\boldsymbol{\eta}(\mathbf{x}, t = 0) = (-1, 0, 0) \quad (4.3)$$

and to

$$\boldsymbol{\eta}(\mathbf{x}, t = 0) = \begin{cases} (-1, 0, 0) & : z > 0 \\ (1, 0, 0) & : z \leq 0, \end{cases} \quad (4.4)$$

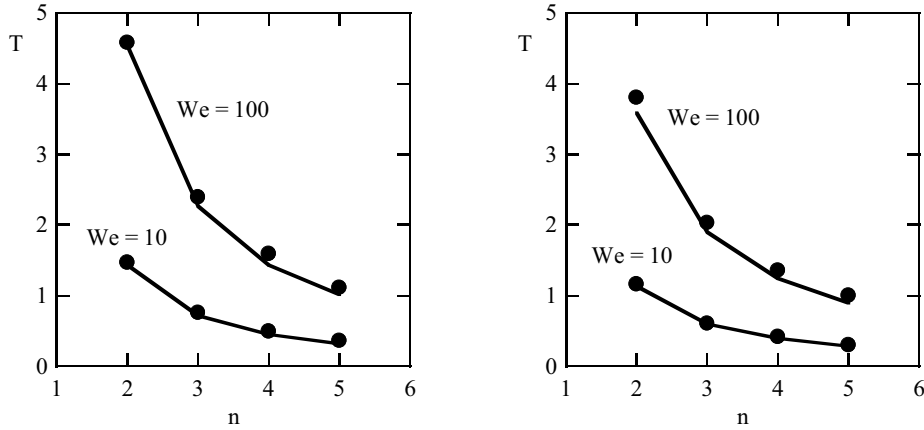


FIGURE 5. Oscillation period T of liquid columns (left) and spheres (right) as a function of mode number n for varying Weber numbers We . Lines denote theoretical and symbols computational results.

in the liquid sheet case. Both, the surface and the sheet simulation were performed in a x - and y -direction periodic box of size $[0, 1] \times [0, 1] \times [-1, 1]$ resolved by a cartesian grid of $64 \times 64 \times 128$ equidistant nodes. In both simulations, the Atwood number is $A = 0$. The Weber number in the surface simulation is $We = 500$ and the Weber number in the sheet simulation based on the sheet thickness is $We_B = 100$.

As depicted in Fig. 6, the surface shows an initial growth of two-dimensional Kelvin-Helmholtz instabilities ($t = 1$). These continue to grow ($t = 3$) and form three-dimensional structures ($t = 5$) resulting in elongated fingers ($t = 6.5$) that finally initiate breakup ($t = 8.0$).

The liquid sheet, depicted in Fig. 7, also exhibits the initial formation of two-dimensional Kelvin-Helmholtz instabilities ($t = 1$) that continue to grow ($t = 3$) until the liquid film gets too thin and ruptures ($t = 5$). Individual fingers are formed that extend mostly in the transverse direction ($t = 8$) and continue to break up into individual drops of varying sizes ($t = 12$).

5. Conclusions and future work

A Eulerian level set/vortex sheet method has been presented that allows for the three-dimensional calculation of the phase interface dynamics between two inviscid and incompressible fluids. Results obtained with the proposed method for oscillating columns and spheres show very good agreement with theoretical predictions. Furthermore, the applicability of the method to the primary breakup process has been demonstrated by simulations of the breakup of both a liquid surface and a liquid sheet.

In addition, the LSS model for turbulent primary breakup has been outlined, and all terms requiring subgrid modeling have been identified. The proposed level set/vortex sheet method has the advantage that it allows for the detailed study of each individual physical process occurring at the phase interface. It thus provides a promising framework for the derivation of the LSS subgrid models.

Future work will focus on including the effect of non-zero Atwood numbers and on coupling of the level set/vortex sheet method to an outside turbulent flow field. Also, the level set/vortex sheet method will be parallelized making use of the new domain decom-

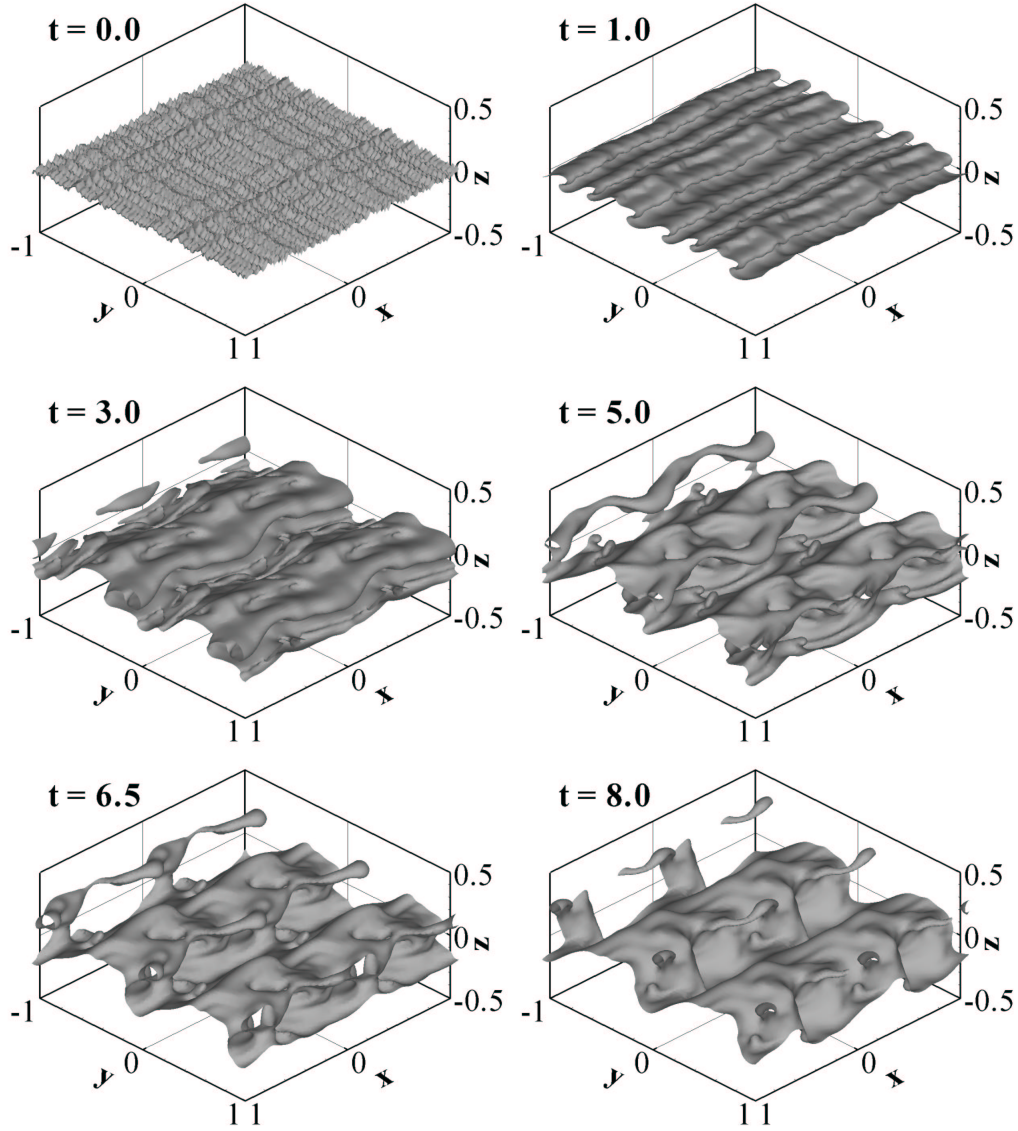


FIGURE 6. Temporal evolution of the three-dimensional liquid surface breakup, $A = 0$, $We = 500$.

position parallelization of the Fast Marching Method presented in Herrmann (2003). This will allow for efficient DNS of the primary breakup process to help identify the different regimes of turbulent primary breakup and their dominant physical processes, facilitating the derivation of the LSS subgrid models. Finally, combining the LSS model to spray models describing the secondary breakup will allow for the first LES of the turbulent atomization process as a whole.

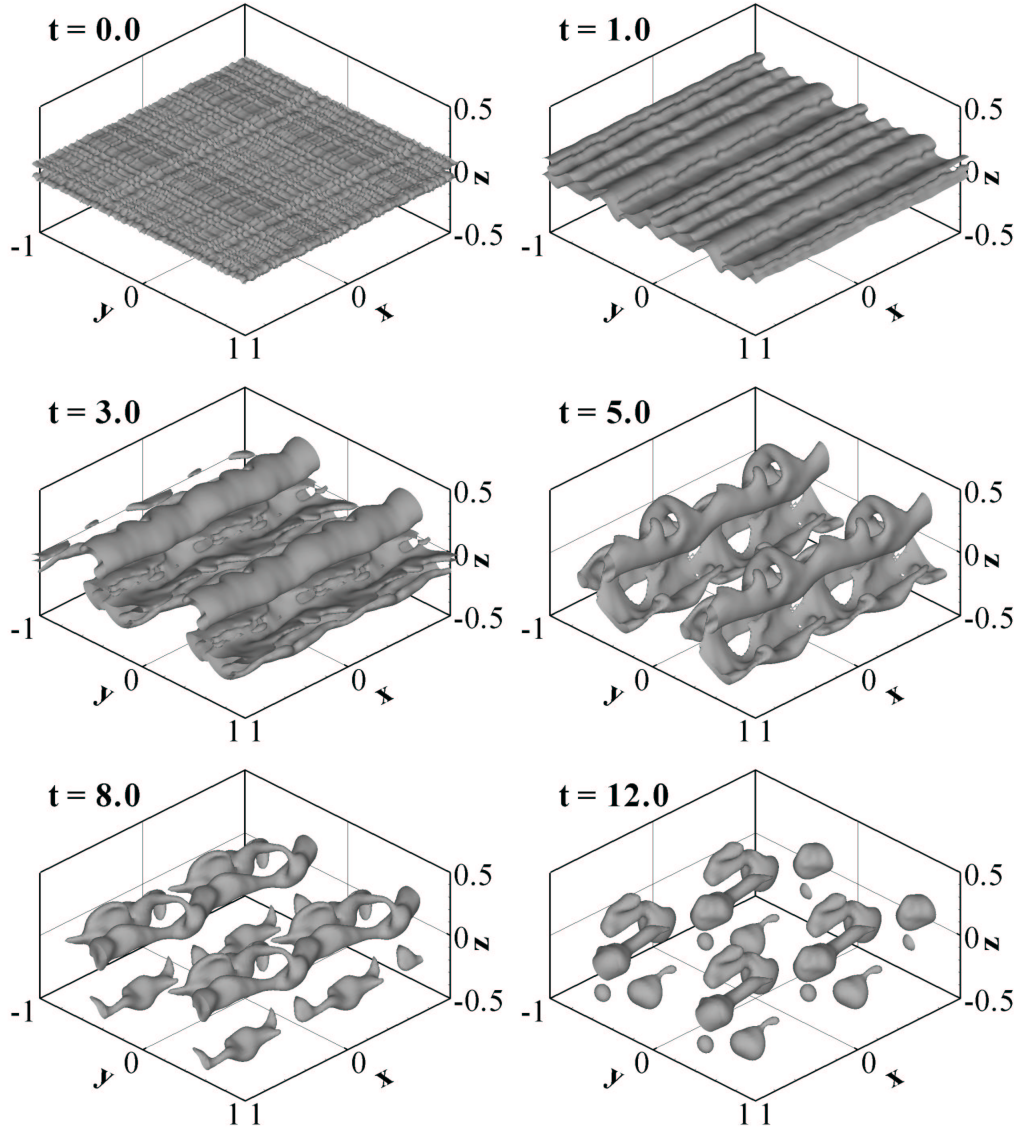


FIGURE 7. Temporal evolution of the three-dimensional liquid sheet breakup, $A = 0$, $We_B = 100$.

Acknowledgments

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